

Isonipecotic acid, N-benzoyl-, hexyl ester

Inchi: InChI=1S/C19H27NO3/c1-2-3-4-8-15-23-19(22)17-11-13-20(14-12-17)18(21)16-9-6-5-7-
InchiKey: SSNJDHMTKQNNCM-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	3.662		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2667.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U360976&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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